



# Mass Spectrometric Instrument for Gaseous and Particulate Characterization



**Developer:** SRI International  
**Contract Number:** DE-AC21-92MC29116  
**Crosscutting Area:** N/A

## Deactivation & Decommissioning FOCUS AREA

### Problem:

Mass spectrometry instruments have been incapable of detecting heavy metals, volatile organic compounds, polynuclear aromatic hydrocarbons, and numerous other pollutants and of detecting a complete mass spectrum from an individual particle. Infrared (IR) spectroscopy and increasing use of chemical microsensors are two approaches suited to situations where only one or several specific compounds are being monitored at any one time. They do not share the versatility of mass spectrometry because of overlapping IR absorptions, or too specific sensor responses to given chemicals. These techniques are not appropriate for the anticipated situation where a great many, potentially unknown and unexpected compounds can be present.

### Solution:

Develop a real time (<1 minute) quantitative, chemical characterization technique for gaseous and particulate pollutants using an ion-trap mass spectrometer. This transportable instrument has a small ion-trap, is lightweight, and operates at a relatively high pressure of 1-2 Pa of Helium (He) buffer gas. This reduces the pumping

requirements and reduces the overall size, complexity, and power requirements of the system. Soft ionization together with the ability to perform mass spectrometry when ambiguities are encountered allows a more immediate response analysis.

### Benefits:

- Real-time quantitative characterization of gaseous & particulate pollutants generated from Department of Energy (DOE) waste cleanup activities
- Detecting and identifying heavy metals, volatile organic compounds, and polynuclear aromatic hydrocarbons
- Designed to operate in the field at any cleanup site
- Provide plant operations with real-time information and alarm capabilities
- Broadly applicable for cleanup or sampling
- High reliability and sensitivity

### Technology:

The instrument was designed with several major components: (1) an

isokinetic sampler capable of operating over a wide range of temperatures (up to 500°K) and flow rates; (2) a high-pressure to low-pressure transition and sampling region that efficiently separates particles from vapor-phase components for separate, parallel analyses; (3) two small mass spectrometers, one optimized for organic analysis using a unique field ionization source and one optimized for particulate characterization using thermal pyrolysis and electron-impact ionization, and (4) a powerful personal computer for control and data acquisition.

The function of the sampler is to obtain a sufficient and representative quantity of air pollutants from a wide range of waste cleanup activities, both vapor and particulate. In addition, the sampler must deliver the vapors and particles to the detection instrument with minimal material loss.

The pressure transition region serves multiple functions: (1) it focuses the particles into a beam toward the center of the gas flow by momentum separation; (2) it efficiently separates the particulate beam from the vapor stream, allowing independent chemical analyses of particles and vapors; and (3) it provides the first



stage of pressure reduction between the ambient atmosphere and the lower pressure (1-2Pa) region of an ion-trap mass spectrometer.

Gaseous compounds are ionized predominantly by use of a rugged field ionization source after enrichment by a membrane separator. Particles are volatilized on a hot filament (~2000°K) and the resulting uncharged vapors are ionized by pulsed electron impact; the timing trigger for the pulsed ionization derives from previous passage through an optical particle counter, which uses light scattering.

### **Project Conclusion:**

The contract was terminated in August 1994 at the end of Phase I because of the lack of obtaining a representative sample for analysis. While there are standard procedures for obtaining representative gaseous samples, representative particulate sampling from an exhaust stream was not achieved. If and when this problem is resolved the system could be an asset to the DOE waste cleanup real time monitoring of emissions.

### **Contacts:**

SRI International performs contract research for industry, government, and foundations in the United States and abroad. Research is conducted in physical and life sciences, economics, management systems, electronics and radio sciences, information science, urban and social systems, and engineering systems. For information on this project, the contractor contact is:

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